

LETTER TO THE EDITOR

Icosahedral multi-component model sets

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Abstract. A quasiperiodic packing \mathcal{Q} of interpenetrating copies of \mathcal{C} , most of them only partially occupied, can be defined in terms of the strip projection method for any icosahedral cluster \mathcal{C} . We show that in the case when the coordinates of the vectors of \mathcal{C} belong to the quadratic field $\mathbb{Q}[\sqrt{5}]$ the dimension of the superspace can be reduced, namely, \mathcal{Q} can be re-defined as a multi-component model set by using a 6-dimensional superspace.

1. Introduction

An icosahedral quasicrystal can be regarded as a quasiperiodic packing of copies of a well-defined icosahedral atomic cluster. Most of these interpenetrating copies are only partially occupied. From a mathematical point of view, an icosahedral cluster \mathcal{C} can be defined as a finite union of orbits of a 3-dimensional representation of the icosahedral group, and there exists an algorithm [2, 3] which leads from \mathcal{C} directly to a pattern \mathcal{Q} which can be regarded as a union of interpenetrating partially occupied translations of \mathcal{C} . This algorithm, based on the strip projection method and group theory, represents an extended version of the model proposed by Katz & Duneau [6] and independently by Elser [5] for the icosahedral quasicrystals.

The dimension of the superspace used in the definition of \mathcal{Q} is rather large, and the main purpose of this paper is to present a way to reduce this dimension. It is based on the notion of *multi-component model set*, an extension of the notion of *model set*, proposed by Baake and Moody [1].

2. Quasiperiodic packings of icosahedral clusters

It is known that the icosahedral group $Y = 235 = \langle a, b \mid a^5 = b^2 = (ab)^3 = e \rangle$ has five irreducible non-equivalent representations and its character table is

	1 e	12 a	15 b	20 ab	12 a^2
Γ_1	1	1	1	1	1
Γ_2	3	τ	-1	0	τ'
Γ_3	3	τ'	-1	0	τ
Γ_4	4	-1	0	1	-1
Γ_5	5	0	1	-1	0

(1)

where $\tau = (1 + \sqrt{5})/2$ and $\tau' = (1 - \sqrt{5})/2$.

A realization of Γ_2 in the usual 3-dimensional Euclidean space $\mathbb{E}_3 = (\mathbb{R}^3, \langle, \rangle)$ is the representation $\{T_g : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 \mid g \in Y\}$ generated by the rotations $T_a, T_b : \mathbb{E}_3 \longrightarrow \mathbb{E}_3$

$$\begin{aligned} T_a(\alpha, \beta, \gamma) &= \left(\frac{\tau-1}{2}\alpha - \frac{\tau}{2}\beta + \frac{1}{2}\gamma, \frac{\tau}{2}\alpha + \frac{1}{2}\beta + \frac{\tau-1}{2}\gamma, -\frac{1}{2}\alpha + \frac{\tau-1}{2}\beta + \frac{\tau}{2}\gamma \right) \\ T_b(\alpha, \beta, \gamma) &= (-\alpha, -\beta, \gamma). \end{aligned} \quad (2)$$

In the case of this representation there are the trivial orbit $Y(0, 0, 0) = \{(0, 0, 0)\}$ of length 1, the orbits

$$Y(\alpha, \alpha\tau, 0) = \{T_g(\alpha, \alpha\tau, 0) \mid g \in Y\} \quad \text{where } \alpha \in (0, \infty) \quad (3)$$

of length 12 (vertices of a regular icosahedron), the orbits

$$Y(\alpha, \alpha, \alpha) = \{T_g(\alpha, \alpha, \alpha) \mid g \in Y\} \quad \text{where } \alpha \in (0, \infty) \quad (4)$$

of length 20 (vertices of a regular dodecahedron), the orbits

$$Y(\alpha, 0, 0) = \{T_g(\alpha, 0, 0) \mid g \in Y\} \quad \text{where } \alpha \in (0, \infty) \quad (5)$$

of length 30 (vertices of an icosidodecahedron), and all the other orbits are of length 60.

Let \mathcal{C} be a fixed icosahedral cluster containing only orbits of length 12, 20 and 30. It can be defined as

$$\mathcal{C} = \bigcup_{x \in S} Yx = \bigcup_{x \in S} \{T_g x \mid g \in Y\} = \{T_g x \mid g \in Y, x \in S\} = YS \quad (6)$$

where the set S contains a representative of each orbit. The entries of the matrices of rotations T_a , T_b in the basis $\{(1, 0, 0), (0, 1, 0), (0, 0, 1)\}$

$$T_a = \frac{1}{2} \begin{pmatrix} \tau - 1 & -\tau & 1 \\ \tau & 1 & \tau - 1 \\ -1 & \tau - 1 & \tau \end{pmatrix} \quad T_b = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (7)$$

belong to the quadratic field $\mathbb{Q}[\sqrt{5}] = \mathbb{Q}[\tau]$. Since $\mathbb{Q}[\tau]$ is dense in \mathbb{R} we can assume that

$$S \subset \{(\alpha, \alpha\tau, 0) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\} \cup \{(\alpha, \alpha, \alpha) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\} \cup \{(\alpha, 0, 0) \mid \alpha \in \mathbb{Q}[\tau], \alpha > 0\}$$

without a significant loss of generality in the description of atomic clusters. Since the orbits of Y of length 12, 20 and 30 are symmetric with respect to the origin, the cluster \mathcal{C} has the form

$$\mathcal{C} = \{e_1, e_2, \dots, e_k, -e_1, -e_2, \dots, -e_k\} \quad (8)$$

and for each vector $e_i = (e_{i1}, e_{i2}, e_{i3})$ the coordinates e_{i1} , e_{i2} , e_{i3} belong to $\mathbb{Q}[\tau]$.

Let $\varepsilon_1 = (1, 0, \dots, 0)$, $\varepsilon_2 = (0, 1, 0, \dots, 0)$, ..., $\varepsilon_k = (0, \dots, 0, 1)$ be the canonical basis of \mathbb{E}_k . For each $g \in Y$, there exist the numbers $s_1^g, s_2^g, \dots, s_k^g \in \{-1; 1\}$ and a permutation of the set $\{1, 2, \dots, k\}$ denoted also by g such that,

$$T_g e_j = s_{g(j)}^g e_{g(j)} \quad \text{for all } j \in \{1, 2, \dots, k\}. \quad (9)$$

Theorem 1. [2, 3] *The formula*

$$g\varepsilon_j = s_{g(j)}^g \varepsilon_{g(j)} \quad (10)$$

defines the orthogonal representation

$$g(x_1, x_2, \dots, x_k) = (s_1^g x_{g^{-1}(1)}, s_2^g x_{g^{-1}(2)}, \dots, s_k^g x_{g^{-1}(k)}) \quad (11)$$

of Y in \mathbb{E}_k .

Theorem 2. [2, 3] *The subspace*

$$E = \{ \langle u, e_1 \rangle, \langle u, e_2 \rangle, \dots, \langle u, e_k \rangle \mid u \in \mathbb{E}_3 \} \quad (12)$$

of \mathbb{E}_k is Y -invariant and the vectors

$$v_1 = \varrho(e_{11}, e_{21}, \dots, e_{k1}) \quad v_2 = \varrho(e_{12}, e_{22}, \dots, e_{k2}) \quad v_3 = \varrho(e_{13}, e_{23}, \dots, e_{k3})$$

where $\varrho = 1/\sqrt{(e_{11})^2 + (e_{21})^2 + \dots + (e_{k1})^2}$ form an orthonormal basis of E .

Theorem 3. [2, 3] *The subduced representation of Y in E is equivalent with the representation of Y in \mathbb{E}_3 , and the isomorphism of representations*

$$\mathcal{I} : \mathbb{E}_3 \longrightarrow E \quad \mathcal{I}u = (\varrho \langle u, e_1 \rangle, \varrho \langle u, e_2 \rangle, \dots, \varrho \langle u, e_k \rangle) \quad (13)$$

with the property $\mathcal{I}(\alpha, \beta, \gamma) = \alpha v_1 + \beta v_2 + \gamma v_3$ allows us to identify the ‘physical’ space \mathbb{E}_3 with the subspace E of \mathbb{E}_k .

Theorem 4. [2, 3] *The matrix of the orthogonal projector $\pi : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ corresponding to E in the basis $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k\}$ is*

$$\pi = \varrho^2 \begin{pmatrix} \langle e_1, e_1 \rangle & \langle e_1, e_2 \rangle & \dots & \langle e_1, e_k \rangle \\ \langle e_2, e_1 \rangle & \langle e_2, e_2 \rangle & \dots & \langle e_2, e_k \rangle \\ \dots & \dots & \dots & \dots \\ \langle e_k, e_1 \rangle & \langle e_k, e_2 \rangle & \dots & \langle e_k, e_k \rangle \end{pmatrix}. \quad (14)$$

Let $\kappa = 1/\varrho$, $\mathbb{L} = \kappa\mathbb{Z}^k$, $\mathbb{K} = [0, \kappa]^k = \{(x_1, x_2, \dots, x_k) \mid 0 \leq x_i \leq \kappa\}$, and let $K = \pi^\perp(\mathbb{K})$, where $\pi^\perp : \mathbb{E}_k \longrightarrow \mathbb{E}_k$, $\pi^\perp x = x - \pi x$ is the orthogonal projector corresponding to the subspace

$$E^\perp = \{x \in \mathbb{E}_k \mid \langle x, y \rangle = 0 \text{ for all } y \in E\}. \quad (15)$$

Theorem 5. [2, 3] *The \mathbb{Z} -module $\mathbb{L} \subset \mathbb{E}_k$ is Y -invariant, $\pi(\kappa\varepsilon_i) = \mathcal{I}e_i$, that is, $\pi(\kappa\varepsilon_i) = e_i$ if we take into consideration the identification $\mathcal{I} : \mathbb{E}_3 \longrightarrow E$, and*

$$\pi(\mathbb{L}) = \mathbb{Z}e_1 + \mathbb{Z}e_2 + \dots + \mathbb{Z}e_k. \quad (16)$$

The pattern defined by using the strip projection method [6]

$$\mathcal{Q} = \{\pi x \mid x \in \mathbb{L}, \pi^\perp x \in K\} \quad (17)$$

can be regarded as a union of interpenetrating copies of \mathcal{C} , most of them only partially occupied. For each point $\pi x \in \mathcal{Q}$ the set of all the arithmetic neighbours of πx

$$\{\pi y \mid y \in \{x + \kappa\varepsilon_1, \dots, x + \kappa\varepsilon_k, x - \kappa\varepsilon_1, \dots, x - \kappa\varepsilon_k\}, \pi^\perp y \in K\}$$

is contained in the translated copy

$$\{\pi x + e_1, \dots, \pi x + e_k, \pi x - e_1, \dots, \pi x - e_k\} = \pi x + \mathcal{C}$$

of the G -cluster \mathcal{C} . The fully occupied clusters occuring in \mathcal{Q} correspond to the points $x \in \mathbb{L}$ satisfying the condition [6]

$$\pi^\perp x \in K \cap \bigcap_{i=1}^k (\pi^\perp(\kappa\varepsilon_i) + K) \cap \bigcap_{i=1}^k (-\pi^\perp(\kappa\varepsilon_i) + K). \quad (18)$$

Generally, only a small part of the clusters occuring in \mathcal{Q} can be fully occupied. A fragment of \mathcal{Q} can be obtained by using, for example, the algorithm presented in [8]. The main difficulty is the rather large dimension k of the superspace \mathbb{E}_k used in the definition of \mathcal{Q} .

3. Icosahedral multi-component model sets

We shall re-define the pattern \mathcal{Q} as a multi-component model set by using a 6-dimensional subspace of \mathbb{E}_k . The automorphism

$$\varphi : \mathbb{Q}[\tau] \longrightarrow \mathbb{Q}[\tau] \quad (19)$$

of the quadratic field $\mathbb{Q}[\tau]$ that maps $\sqrt{5} \mapsto -\sqrt{5}$ has the property $\varphi(\tau) = \tau'$. The representation (2) is related through φ to the representation $\{T'_g : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 \mid g \in Y\}$ belonging to Γ_3 generated by the rotations $T'_a, T'_b : \mathbb{E}_3 \longrightarrow \mathbb{E}_3$

$$\begin{aligned} T'_a(\alpha, \beta, \gamma) &= \left(\frac{\tau'-1}{2}\alpha - \frac{\tau'}{2}\beta + \frac{1}{2}\gamma, \frac{\tau'}{2}\alpha + \frac{1}{2}\beta + \frac{\tau'-1}{2}\gamma, -\frac{1}{2}\alpha + \frac{\tau'-1}{2}\beta + \frac{\tau'}{2}\gamma \right) \\ T'_b(\alpha, \beta, \gamma) &= (-\alpha, -\beta, \gamma). \end{aligned} \quad (20)$$

If instead of the representation (2) and cluster \mathcal{C} we start from the representation (20) and the cluster

$$\mathcal{C}' = \{e'_1, e'_2, \dots, e'_k, -e'_1, -e'_2, \dots, -e'_k\} \quad (21)$$

where

$$e'_i = (e'_{i1}, e'_{i2}, e'_{i3}) = (\varphi(e_{i1}), \varphi(e_{i2}), \varphi(e_{i3})) \quad (22)$$

then we get the same representation of Y in \mathbb{E}_k and the Y -invariant subspace

$$E' = \{ \langle u, e'_1 \rangle, \langle u, e'_2 \rangle, \dots, \langle u, e'_k \rangle \mid u \in \mathbb{E}_3 \}. \quad (23)$$

The vectors

$$v'_1 = \varrho'(e'_{11}, e'_{21}, \dots, e'_{k1}) \quad v'_2 = \varrho'(e'_{12}, e'_{22}, \dots, e'_{k2}) \quad v'_3 = \varrho'(e'_{13}, e'_{23}, \dots, e'_{k3})$$

where $\varrho' = 1/\sqrt{(e'_{11})^2 + (e'_{21})^2 + \dots + (e'_{k1})^2}$, form an orthonormal basis of E' , and the matrix of the orthogonal projector $\pi' : \mathbb{E}_k \longrightarrow \mathbb{E}_k$ corresponding to E' in the basis $\{\varepsilon_1, \varepsilon_2, \dots, \varepsilon_k\}$ is

$$\pi' = \varrho'^2 \begin{pmatrix} \langle e'_1, e'_1 \rangle & \langle e'_1, e'_2 \rangle & \dots & \langle e'_1, e'_k \rangle \\ \langle e'_2, e'_1 \rangle & \langle e'_2, e'_2 \rangle & \dots & \langle e'_2, e'_k \rangle \\ \dots & \dots & \dots & \dots \\ \langle e'_k, e'_1 \rangle & \langle e'_k, e'_2 \rangle & \dots & \langle e'_k, e'_k \rangle \end{pmatrix}. \quad (24)$$

Theorem 6. *The projectors π and π' are orthogonal, that is,*

$$\pi\pi' = \pi'\pi = 0$$

and the projector $\pi + \pi'$ corresponding to the subspace $\mathcal{E} = E \oplus E'$ has rational entries.

Proof. Consider the linear mapping

$$A : \mathbb{E}_3 \longrightarrow \mathbb{E}_3 : u \mapsto Au \quad \text{where} \quad Au = \sum_{i=1}^k \langle u, e_i \rangle e'_i.$$

Since A is a morphism of representations

$$\begin{aligned} A(T_g u) &= \sum_{i=1}^k \langle T_g u, e_i \rangle e'_i = \sum_{i=1}^k \langle u, T_g^{-1} e_i \rangle e'_i \\ &= T'_g \left(\sum_{i=1}^k \langle u, T_g^{-1} e_i \rangle T'^{-1}_g e'_i \right) = T'_g \left(\sum_{i=1}^k \langle u, e_i \rangle e'_i \right) = T'_g(Au) \end{aligned}$$

between the irreducible non-equivalent representations (2) and (20), from Schur's lemma it follows that $A = 0$, that is, $\sum_{i=1}^k \langle u, e_i \rangle e'_i = 0$ for any $u \in \mathbb{E}_3$. Particularly, we have

$$\sum_{i=1}^k \langle e_j, e_i \rangle \langle e'_i, e'_l \rangle = \langle \sum_{i=1}^k \langle e_j, e_i \rangle e'_i, e'_l \rangle = 0$$

whence $\pi\pi' = 0$. In a similar way we can prove that $\pi'\pi = 0$. Since

$$\varrho'^2 \langle e'_i, e'_j \rangle = \varphi(\varrho^2 \langle e_i, e_j \rangle)$$

we get $\varrho'^2 \langle e'_i, e'_j \rangle + \varrho^2 \langle e_i, e_j \rangle \in \mathbb{Q}$, that is, the projector $\pi + \pi'$ has rational entries.

Theorem 7. *The collection of spaces and mappings*

$$\begin{array}{c} \pi x \leftarrow x : E \xleftarrow{\pi} \mathcal{E} \xrightarrow{\pi'} E' : x \rightarrow \pi' x \\ \cup \\ \mathcal{L} \end{array} \quad (25)$$

where $\mathcal{L} = (\pi + \pi')(\mathbb{L})$, is a cut and project scheme [1, 7].

Proof. Since, in view of theorem 5, we have

$$\pi'(\mathcal{L}) = \pi'(\pi + \pi')(\mathbb{L}) = \pi'(\mathbb{L}) = \sum_{i=1}^k \mathbb{Z}e'_i$$

the set $\pi'(\mathcal{L})$ is dense in E' . For each $x \in \mathcal{L}$ there is $\kappa y \in \mathbb{L}$ with $y \in \mathbb{Z}^k$ such that $x = (\pi + \pi')(\kappa y)$. If $\pi x = 0$ then $\pi(\pi + \pi')(\kappa y) = 0$, whence $\pi(\kappa y) = 0$. But, $\pi(\kappa y) = \kappa\pi y$, and hence we have $\pi y = 0$. Since $y \in \mathbb{Z}^k$, from $\pi y = 0$ we get $\pi' y = 0$, whence $x = (\pi + \pi')y = 0$. This means that π restricted to \mathcal{L} is injective.

Let $E'' = \mathcal{E}^\perp = \{x \in \mathbb{E}_k \mid \langle x, y \rangle = 0 \text{ for all } y \in \mathcal{E}\}$ and let $\pi'' : \mathbb{E}_k \longrightarrow \mathbb{E}_k$, $\pi''x = x - \pi x - \pi'x$ be the corresponding orthogonal projector. The lattice $L = \mathbb{L} \cap \mathcal{E}$ is a sublattice of \mathcal{L} , and necessarily $[\mathcal{L} : L]$ is finite. Since π'' has rational entries the projection $\mathbb{L}'' = \pi''(\mathbb{L})$ of \mathbb{L} on E'' is a discrete countable set. Let $\mathcal{Z} = \{z_i \mid i \in \mathbb{Z}\}$ be a subset of \mathbb{L} such that $\mathbb{L}'' = \pi''(\mathcal{Z})$ and $\pi''z_i \neq \pi''z_j$ for $i \neq j$. The lattice \mathbb{L} is contained in the union of the cosets $\mathcal{E}_i = z_i + \mathcal{E} = \{z_i + x \mid x \in \mathcal{E}\}$

$$\mathbb{L} \subset \bigcup_{i \in \mathbb{Z}} \mathcal{E}_i. \quad (26)$$

Since $\mathbb{L} \cap \mathcal{E}_i = z_i + L$ the set

$$\mathcal{L}_i = (\pi + \pi')(\mathbb{L} \cap \mathcal{E}_i) = (\pi + \pi')z_i + L \quad (27)$$

is a coset of L in \mathcal{L} for any $i \in \mathbb{Z}$.

Only for a finite number of cosets \mathcal{E}_i the intersection

$$K_i = K \cap \mathcal{E}_i = \pi^\perp(\mathbb{K} \cap \mathcal{E}_i) \subset \pi''z_i + E' \quad (28)$$

is non-empty. By changing the indexation of the elements of \mathcal{Z} if necessary, we can assume that the subset of E'

$$\mathcal{K}_i = \pi'(K_i) = \pi'(\mathbb{K} \cap \mathcal{E}_i) \subset E' \quad (29)$$

has a non-empty interior only for $i \in \{1, \dots, m\}$. The ‘polyhedral’ set \mathcal{K}_i satisfies the conditions:

- (a) $\mathcal{K}_i \subset E'$ is compact;
- (b) $\mathcal{K}_i = \overline{\text{int}(\mathcal{K}_i)}$;
- (c) The boundary of \mathcal{K}_i has Lebesgue measure 0

for any $i \in \{1, \dots, m\}$. This allows us to re-define \mathcal{Q} in terms of the 6-dimensional superspace \mathcal{E} as a multi-component model set [1]

$$\mathcal{Q} = \bigcup_{i=1}^m \{ \pi x \mid x \in \mathcal{L}_i, \pi' x \in \mathcal{K}_i \}. \quad (30)$$

It is known [4] that this is the minimal embedding for a 3-dimensional quasiperiodic point set with icosahedral symmetry. The main difficulty in this new approach is the determination of the ‘atomic surfaces’ \mathcal{K}_i .

Acknowledgments

This research was supported by the grant CNCSIS no. 630/2003.

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